

Neutron Reflectivity from Biomimetic Membranes: Improving Reliability through Wavelet Analysis

Understanding such key biological processes as molecular recognition, protein insertion, and molecular self-assembly in *living* biological membranes remains a challenge. Membrane materials mimicking biological ones (biomimetic membranes) provide model systems to address this issue, and, because of its special sensitivity to hydrogen, neutron reflectivity (NR) offers a unique way to reveal thin film structures in biomimetic membranes.

The feasibility of using phase-inversion techniques in NR to reveal such structural details has been demonstrated [1]. It is possible to directly measure the real part, $r_I(Q)$, of the complex reflection coefficient $r(Q)$ as a function of wavevector Q and to mathematically invert it to obtain the

scattering length density (SLD) depth profile $\rho(x)$ of the film. There remains much to do, however, in defining the reliability of the results, especially in accessing the unavoidable reduction of spatial resolution induced by data truncated at a maximum wavevector, Q_{max} . Wavelet analysis provides a systematic and useful approach to the problem [2].

In using Wavelet MultiResolution Analysis (WMRA), SLD profiles are characterized by a finest length scale $\ell_0 \approx 1 \text{ \AA}$ and coarser scales, $\ell_j = 2^{-j}\ell_0$, with j negative. $\rho(x)$ viewed as a coarse “trend” $\rho_f(x)$ at resolution level J , with added “detail” $\Delta_j\rho(x)$ giving the trend at the next finer scale, $\rho_{j+1}(x) = \rho_f(x) + \Delta_j\rho(x)$. Relative to a base scale of resolution ℓ_j , the SLD profile thus can be represented by the trend plus all remaining detail, $\rho(x) = \rho_j(x) + \sum_{j=J}^{\infty} \Delta_j\rho(x)$. The experimental $\rho(x)$, associated with a given Q_{max} determined by the instrument, is a blurred representation of the veridical SLD. It can be thought of as a coarse image bracketed by neighboring trends for this Q_{max} .

WMRA provides spatially localized orthonormal bases for this description. A family of wavelets called Daubechies-8 seems well suited to NR analysis. For illustration, we use a realistic SLD profile obtained by molecular modeling to represent a hybrid lipid membrane on a thin gold film (diagram on top of Fig. 1), a biomimetic system typical of those being studied in many laboratories. The model $\rho(x)$, seen in the back panes of Figs. 1 and 2, consists of the gold layer, a hydrogenated alkanethiol layer, and a deuterated lipid monolayer.

Figures 1 and 2 depict the convergence of the WMRA descriptions of $\rho(x)$ as trend and detail. The “overall” shape of $\rho(x)$ effectively is determined by the trend $\rho_4(x)$ and detail $\Delta_4\rho(x)$, *i.e.*, by trend $\rho_3(x)$. However, emergence of the prominent double peaked structure of the lipid head group near $x/l_0 = 100$ needs detail $\Delta_3\rho(x)$. Subsequent detail mainly acts to sharpen the edges between the film’s components.

Figure 3 shows the effective contributions of the trend and the successive spatial detail to the reflection coefficient $r(Q)$, each calculated exactly. The edge-sharpening detail seen in Fig. 3 is not revealed in the reflection spectrum below $Q\ell_0 \approx 0.6$. Figure 4 shows the “smeared” $\rho(x)$ obtained by direct inversion of the reflec-

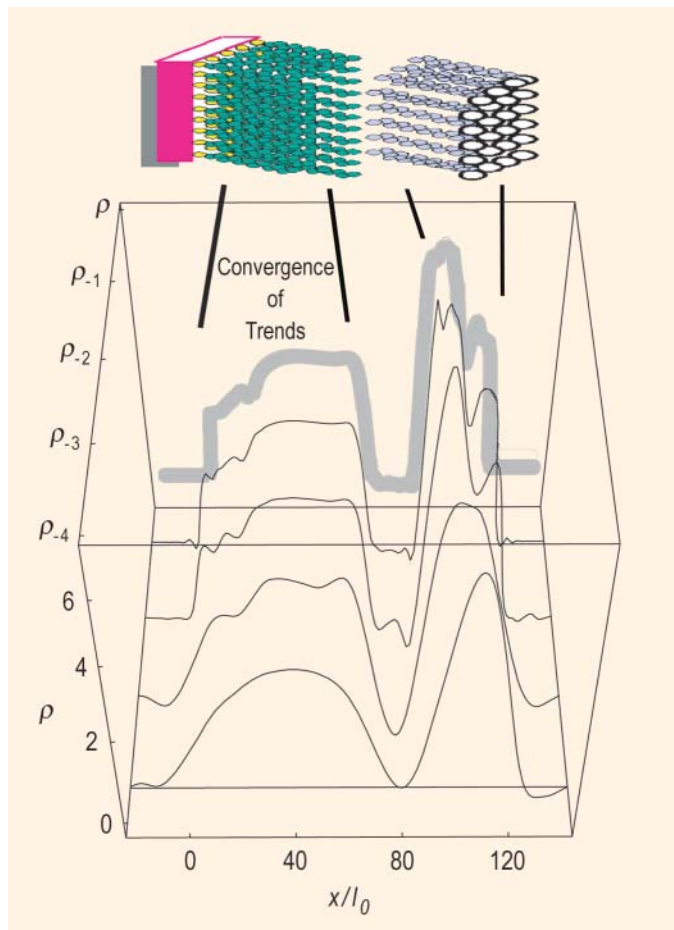


Fig. 1. Diagram of model (top) for which the computed scattering length density $\rho(x)$ is the thick grey curve. Trends converge: $\rho_4(x)$, $\rho_3(x)$, $\dots \rightarrow \rho(x)$.

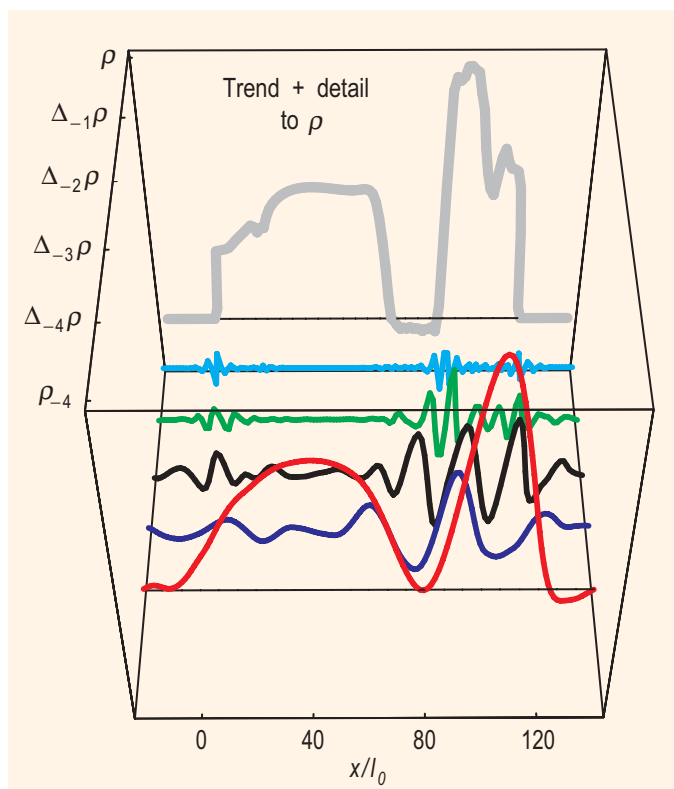


Fig. 2. Trend plus detail converges: $\rho_{-4}(x) + \Delta_{-4}\rho(x) + \Delta_{-3}\rho(x), \dots \rightarrow \rho(x)$.

tion from $\rho(x)$ using data truncated at $Q_{\max} \approx 0.2 \text{ \AA}^{-1}$. This is seen to fall “between” the trends $\rho_{-4}(x)$ and $\rho_{-3}(x)$, stemming from low-pass filters with roll-offs at $Q \approx 0.2 \text{ \AA}^{-1}$ and $Q \approx 0.4 \text{ \AA}^{-1}$, respectively. This is expected from the fact that the Fourier transforms of trends and detail overlap to a degree. Thus, a “pure” trend cannot be observed in the truncated data.

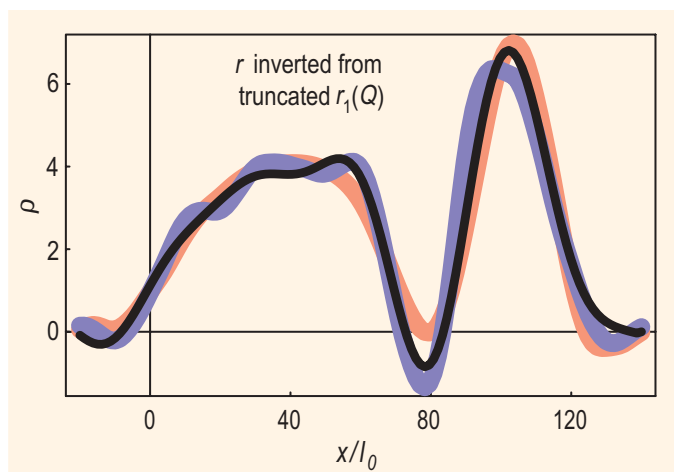


Fig. 4. Inverted $r_1(Q)$ (black) using only data truncated at $Ql_0 = 0.2$. Trends $\rho_{-4}(x)$ (red) and $\rho_{-3}(x)$ (blue) of the actual $\rho(x)$.

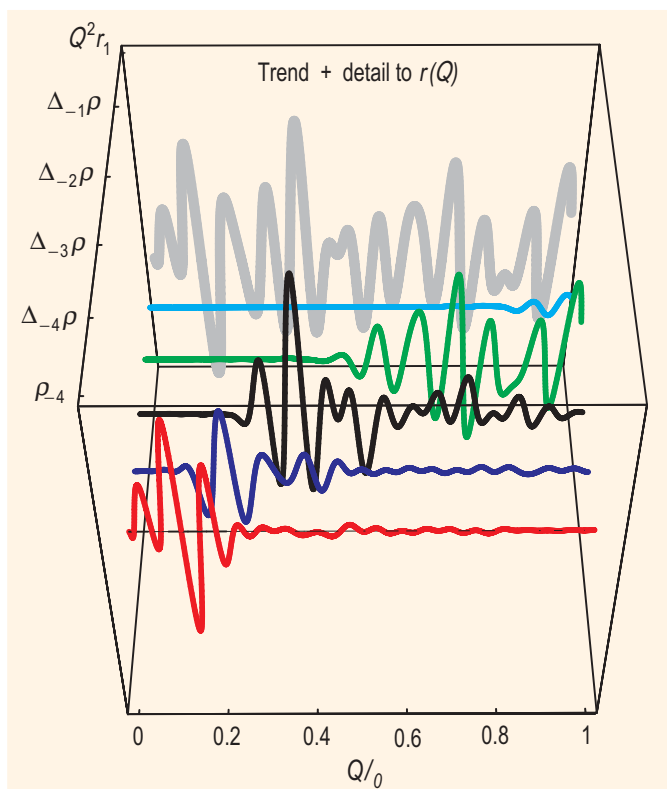


Fig. 3. Effective contributions to $Q^2 r_1(Q)$ generated by the trend $\rho_{-4}(x)$ (in red) and the details $\Delta_j \rho(x)$ for $j = -4, -3, -2, -1$ shown in Fig. 2. The $Q^2 r_1(Q)$ contributions are labeled by the SLD's that produced them.

Wavelet analysis thus provides a systematic method for assessing the correctness of density profiles measured by NR. It promises to add reliability in unraveling structures of importance in biomimetic membranes.

References:

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